



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 06:26 PM UTC

PDB ID : 8JZQ / pdb_00008jzq
Title : Crystal structure of Panax quinquefolius Pq3-O-UGT2
Authors : Mei, K.; Ji, Q.; Liu, Y.
Deposited on : 2023-07-06
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

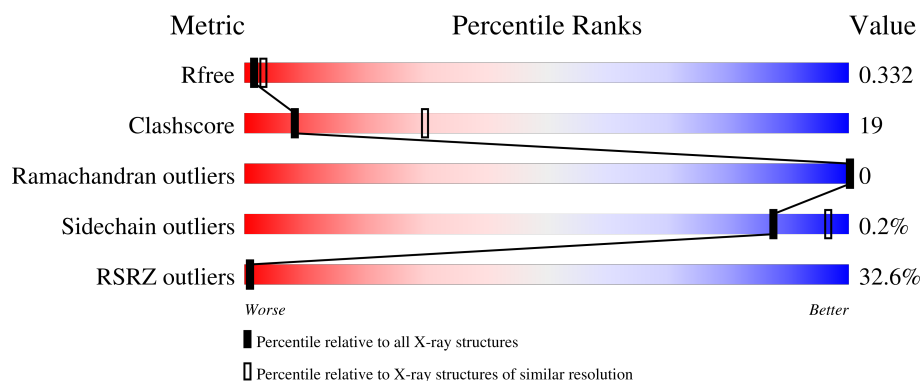
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	455	17% 64% 18% • 17%
1	B	455	28% 64% 19% 17%
1	C	455	30% 64% 19% 17%
1	D	455	33% 64% 19% 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11872 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2968	1902	500	554	12			
1	B	378	Total	C	N	O	S	0	0	0
			2968	1902	500	554	12			
1	C	378	Total	C	N	O	S	0	0	0
			2968	1902	500	554	12			
1	D	378	Total	C	N	O	S	0	0	0
			2968	1902	500	554	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	443	GLU	-	expression tag	UNP A0A0M4ME80
A	444	ASN	-	expression tag	UNP A0A0M4ME80
A	445	LEU	-	expression tag	UNP A0A0M4ME80
A	446	TYR	-	expression tag	UNP A0A0M4ME80
A	447	PHE	-	expression tag	UNP A0A0M4ME80
A	448	GLN	-	expression tag	UNP A0A0M4ME80
A	449	GLY	-	expression tag	UNP A0A0M4ME80
A	450	HIS	-	expression tag	UNP A0A0M4ME80
A	451	HIS	-	expression tag	UNP A0A0M4ME80
A	452	HIS	-	expression tag	UNP A0A0M4ME80
A	453	HIS	-	expression tag	UNP A0A0M4ME80
A	454	HIS	-	expression tag	UNP A0A0M4ME80
A	455	HIS	-	expression tag	UNP A0A0M4ME80
B	443	GLU	-	expression tag	UNP A0A0M4ME80
B	444	ASN	-	expression tag	UNP A0A0M4ME80
B	445	LEU	-	expression tag	UNP A0A0M4ME80
B	446	TYR	-	expression tag	UNP A0A0M4ME80
B	447	PHE	-	expression tag	UNP A0A0M4ME80
B	448	GLN	-	expression tag	UNP A0A0M4ME80
B	449	GLY	-	expression tag	UNP A0A0M4ME80
B	450	HIS	-	expression tag	UNP A0A0M4ME80

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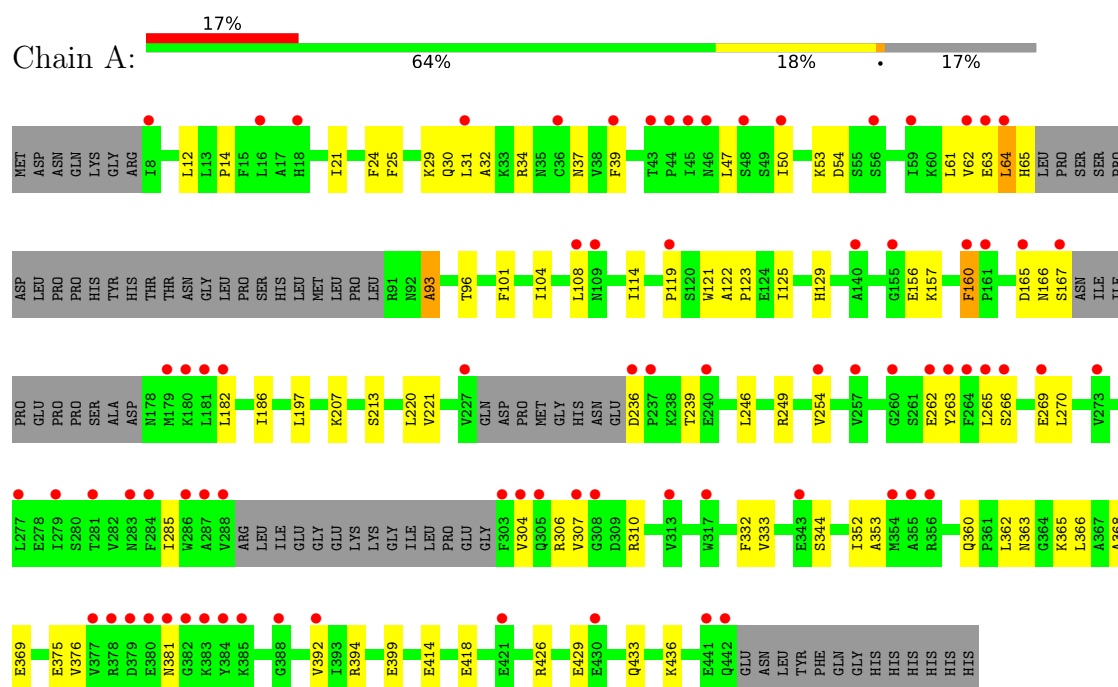
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Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	expression tag	UNP A0A0M4ME80
B	452	HIS	-	expression tag	UNP A0A0M4ME80
B	453	HIS	-	expression tag	UNP A0A0M4ME80
B	454	HIS	-	expression tag	UNP A0A0M4ME80
B	455	HIS	-	expression tag	UNP A0A0M4ME80
C	443	GLU	-	expression tag	UNP A0A0M4ME80
C	444	ASN	-	expression tag	UNP A0A0M4ME80
C	445	LEU	-	expression tag	UNP A0A0M4ME80
C	446	TYR	-	expression tag	UNP A0A0M4ME80
C	447	PHE	-	expression tag	UNP A0A0M4ME80
C	448	GLN	-	expression tag	UNP A0A0M4ME80
C	449	GLY	-	expression tag	UNP A0A0M4ME80
C	450	HIS	-	expression tag	UNP A0A0M4ME80
C	451	HIS	-	expression tag	UNP A0A0M4ME80
C	452	HIS	-	expression tag	UNP A0A0M4ME80
C	453	HIS	-	expression tag	UNP A0A0M4ME80
C	454	HIS	-	expression tag	UNP A0A0M4ME80
C	455	HIS	-	expression tag	UNP A0A0M4ME80
D	443	GLU	-	expression tag	UNP A0A0M4ME80
D	444	ASN	-	expression tag	UNP A0A0M4ME80
D	445	LEU	-	expression tag	UNP A0A0M4ME80
D	446	TYR	-	expression tag	UNP A0A0M4ME80
D	447	PHE	-	expression tag	UNP A0A0M4ME80
D	448	GLN	-	expression tag	UNP A0A0M4ME80
D	449	GLY	-	expression tag	UNP A0A0M4ME80
D	450	HIS	-	expression tag	UNP A0A0M4ME80
D	451	HIS	-	expression tag	UNP A0A0M4ME80
D	452	HIS	-	expression tag	UNP A0A0M4ME80
D	453	HIS	-	expression tag	UNP A0A0M4ME80
D	454	HIS	-	expression tag	UNP A0A0M4ME80
D	455	HIS	-	expression tag	UNP A0A0M4ME80

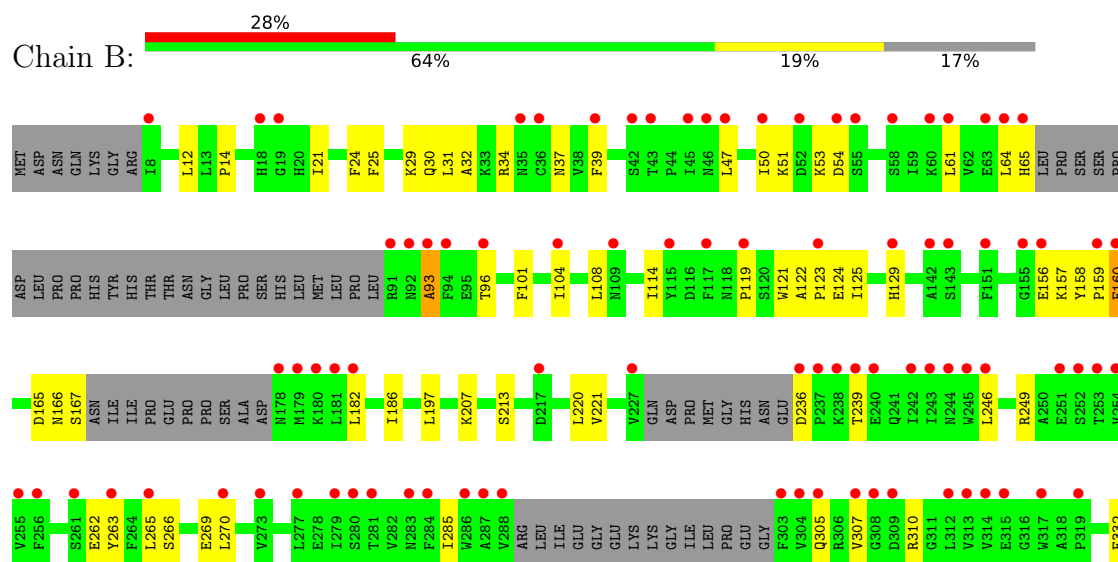
3 Residue-property plots [i](#)

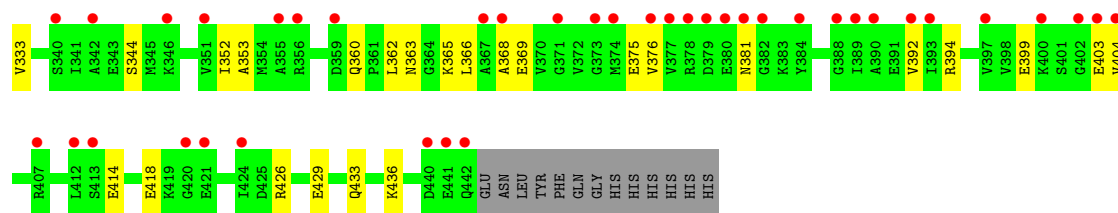
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glycosyltransferase

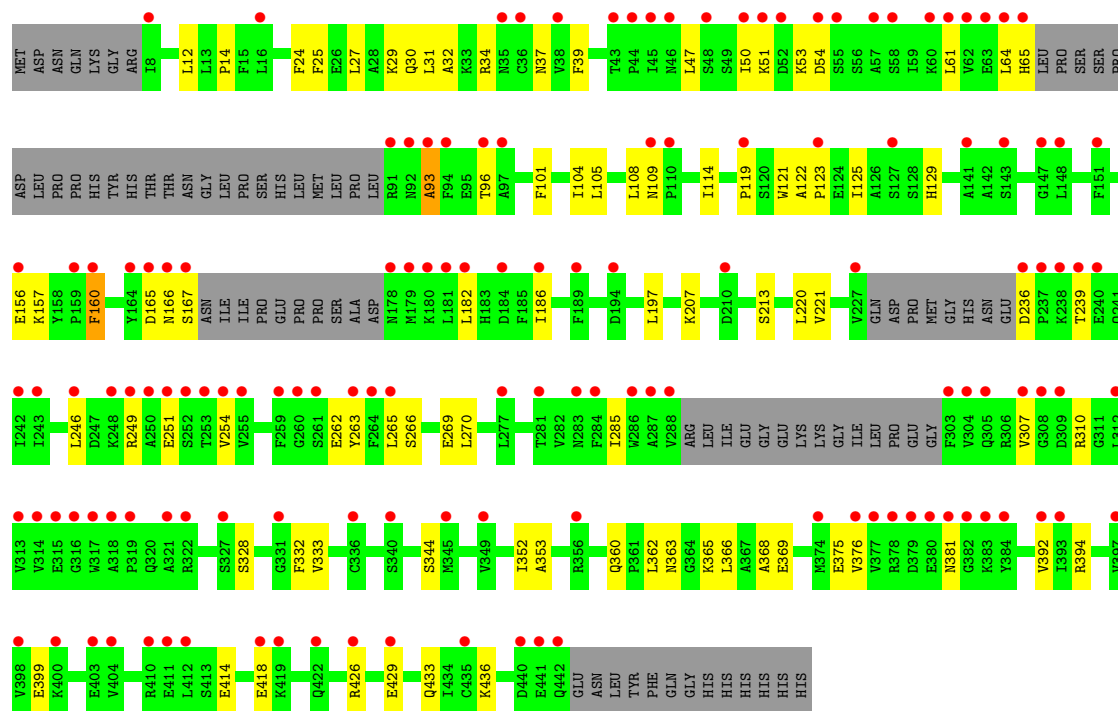


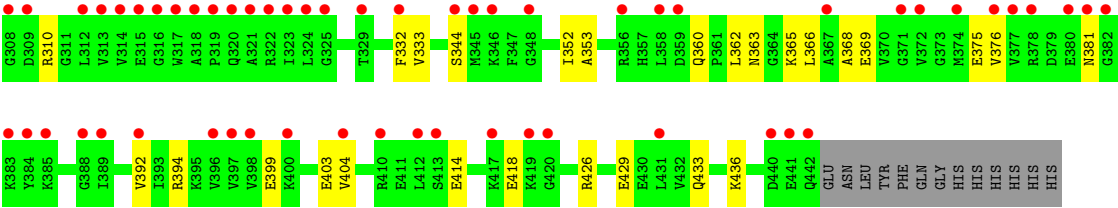
• Molecule 1: Glycosyltransferase





• Molecule 1: Glycosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.99Å 80.89Å 126.38Å 93.96° 90.00° 93.75°	Depositor
Resolution (Å)	37.70 – 2.89 37.70 – 2.89	Depositor EDS
% Data completeness (in resolution range)	94.3 (37.70-2.89) 94.5 (37.70-2.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.307 , 0.333 0.306 , 0.332	Depositor DCC
R_{free} test set	1930 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	11872	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/3027	0.85	3/4086 (0.1%)
1	B	0.55	0/3027	0.84	3/4086 (0.1%)
1	C	0.55	0/3027	0.84	3/4086 (0.1%)
1	D	0.55	0/3027	0.84	3/4086 (0.1%)
All	All	0.55	0/12108	0.84	12/16344 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	ASN	N-CA-C	-5.74	108.08	114.62
1	C	381	ASN	N-CA-C	-5.74	108.08	114.62
1	D	381	ASN	N-CA-C	-5.71	108.10	114.62
1	A	381	ASN	N-CA-C	-5.71	108.11	114.62
1	A	160	PHE	CA-C-O	-5.63	113.67	120.08
1	B	160	PHE	CA-C-O	-5.61	113.69	120.08
1	D	160	PHE	CA-C-O	-5.60	113.70	120.08
1	C	160	PHE	CA-C-O	-5.58	113.72	120.08
1	D	93	ALA	N-CA-C	-5.28	106.67	113.01
1	C	93	ALA	N-CA-C	-5.26	106.70	113.01
1	B	93	ALA	N-CA-C	-5.25	106.70	113.01
1	A	93	ALA	N-CA-C	-5.22	106.75	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2968	0	2984	115	7
1	B	2968	0	2984	111	10
1	C	2968	0	2984	115	6
1	D	2968	0	2983	115	8
All	All	11872	0	11935	456	27

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (456) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LEU:HD11	1:B:269:GLU:CB	1.07	1.54
1:C:265:LEU:HD11	1:C:269:GLU:CB	1.07	1.54
1:B:265:LEU:CD1	1:B:269:GLU:CB	1.87	1.52
1:D:265:LEU:CD1	1:D:269:GLU:CB	1.87	1.52
1:D:265:LEU:HD11	1:D:269:GLU:CB	1.07	1.51
1:A:265:LEU:HD11	1:A:269:GLU:CB	1.07	1.50
1:A:265:LEU:CD1	1:A:269:GLU:HB2	1.40	1.50
1:C:265:LEU:CD1	1:C:269:GLU:CB	1.87	1.50
1:C:265:LEU:CG	1:C:269:GLU:HB2	1.41	1.50
1:B:265:LEU:CD1	1:B:269:GLU:HB2	1.40	1.49
1:A:265:LEU:CD1	1:A:269:GLU:CB	1.87	1.49
1:D:265:LEU:CD1	1:D:269:GLU:HB2	1.40	1.49
1:B:265:LEU:CG	1:B:269:GLU:HB2	1.41	1.47
1:A:265:LEU:CG	1:A:269:GLU:HB2	1.41	1.47
1:D:265:LEU:CG	1:D:269:GLU:HB2	1.41	1.47
1:C:265:LEU:CD1	1:C:269:GLU:HB2	1.40	1.46
1:A:265:LEU:HD21	1:A:269:GLU:C	1.44	1.42
1:B:265:LEU:HD21	1:B:269:GLU:C	1.44	1.42
1:A:37:ASN:HB2	1:A:39:PHE:CZ	1.56	1.40
1:D:265:LEU:HD21	1:D:269:GLU:C	1.44	1.40
1:D:37:ASN:HB2	1:D:39:PHE:CZ	1.56	1.40
1:C:265:LEU:HD21	1:C:269:GLU:C	1.44	1.39
1:C:37:ASN:HB2	1:C:39:PHE:CZ	1.56	1.38
1:B:37:ASN:HB2	1:B:39:PHE:CZ	1.56	1.38
1:B:32:ALA:HA	1:B:39:PHE:CE2	1.63	1.34
1:D:32:ALA:HA	1:D:39:PHE:CE2	1.63	1.31
1:C:32:ALA:HA	1:C:39:PHE:CE2	1.63	1.31
1:A:32:ALA:HA	1:A:39:PHE:CE2	1.63	1.30
1:D:265:LEU:HD11	1:D:269:GLU:CG	1.65	1.27
1:A:265:LEU:HD11	1:A:269:GLU:CG	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:LEU:HD11	1:C:269:GLU:CG	1.65	1.25
1:B:265:LEU:HD11	1:B:269:GLU:CG	1.65	1.25
1:A:262:GLU:OE1	1:A:360:GLN:NE2	1.81	1.14
1:B:262:GLU:OE1	1:B:360:GLN:NE2	1.81	1.13
1:D:262:GLU:OE1	1:D:360:GLN:NE2	1.81	1.12
1:C:262:GLU:OE1	1:C:360:GLN:NE2	1.81	1.11
1:A:157:LYS:HZ2	1:A:166:ASN:N	1.48	1.11
1:A:265:LEU:CD2	1:A:269:GLU:C	2.25	1.10
1:D:265:LEU:CD2	1:D:269:GLU:C	2.25	1.10
1:B:265:LEU:HG	1:B:266:SER:H	1.15	1.10
1:C:265:LEU:CD2	1:C:269:GLU:C	2.25	1.09
1:B:265:LEU:CD2	1:B:269:GLU:C	2.25	1.08
1:C:265:LEU:HG	1:C:266:SER:H	1.15	1.08
1:A:265:LEU:HG	1:A:266:SER:H	1.15	1.08
1:B:265:LEU:HD11	1:B:269:GLU:HB3	1.07	1.06
1:D:265:LEU:HG	1:D:266:SER:H	1.15	1.06
1:D:265:LEU:HG	1:D:269:GLU:HB2	1.36	1.06
1:B:265:LEU:HG	1:B:269:GLU:HB2	1.36	1.05
1:C:265:LEU:HD11	1:C:269:GLU:HB3	1.07	1.05
1:D:265:LEU:HD11	1:D:269:GLU:HB3	1.07	1.04
1:A:265:LEU:HD11	1:A:269:GLU:HB3	1.07	1.02
1:B:37:ASN:O	1:B:39:PHE:CE2	2.13	1.02
1:C:37:ASN:O	1:C:39:PHE:CE2	2.13	1.02
1:A:265:LEU:HG	1:A:269:GLU:HB2	1.36	1.02
1:D:37:ASN:O	1:D:39:PHE:CE2	2.13	1.02
1:C:265:LEU:HG	1:C:269:GLU:HB2	1.36	1.01
1:A:32:ALA:CA	1:A:39:PHE:CE2	2.43	1.01
1:A:37:ASN:O	1:A:39:PHE:CE2	2.13	1.01
1:C:37:ASN:O	1:C:39:PHE:CD2	2.14	1.01
1:C:32:ALA:CA	1:C:39:PHE:CE2	2.43	1.01
1:B:37:ASN:O	1:B:39:PHE:CD2	2.14	1.01
1:D:32:ALA:CA	1:D:39:PHE:CE2	2.43	1.01
1:D:37:ASN:O	1:D:39:PHE:CD2	2.14	1.00
1:B:32:ALA:CA	1:B:39:PHE:CE2	2.43	1.00
1:A:37:ASN:O	1:A:39:PHE:CD2	2.14	1.00
1:B:157:LYS:HZ2	1:B:166:ASN:N	1.58	0.99
1:C:265:LEU:CG	1:C:269:GLU:CB	2.30	0.98
1:A:157:LYS:HZ3	1:A:167:SER:H	1.12	0.98
1:B:265:LEU:HD21	1:B:269:GLU:CA	1.95	0.97
1:C:265:LEU:HD21	1:C:269:GLU:CA	1.95	0.97
1:B:265:LEU:CG	1:B:269:GLU:CB	2.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:LYS:HZ2	1:C:166:ASN:N	1.62	0.96
1:A:265:LEU:HD21	1:A:269:GLU:CA	1.95	0.96
1:D:157:LYS:HZ2	1:D:166:ASN:N	1.64	0.96
1:D:265:LEU:HD21	1:D:269:GLU:CA	1.95	0.95
1:A:265:LEU:HD21	1:A:269:GLU:CB	1.97	0.95
1:A:157:LYS:HZ2	1:A:166:ASN:H	1.04	0.94
1:C:31:LEU:O	1:C:39:PHE:HZ	1.51	0.94
1:D:37:ASN:CB	1:D:39:PHE:CZ	2.50	0.94
1:A:37:ASN:CB	1:A:39:PHE:CZ	2.50	0.94
1:C:265:LEU:HD21	1:C:269:GLU:CB	1.97	0.94
1:B:265:LEU:HD21	1:B:269:GLU:CB	1.97	0.93
1:B:31:LEU:O	1:B:39:PHE:CZ	2.22	0.93
1:B:31:LEU:O	1:B:39:PHE:HZ	1.51	0.93
1:B:32:ALA:HA	1:B:39:PHE:HE2	1.04	0.93
1:D:31:LEU:O	1:D:39:PHE:CZ	2.22	0.93
1:A:265:LEU:CG	1:A:269:GLU:CB	2.30	0.93
1:D:265:LEU:HD21	1:D:269:GLU:CB	1.97	0.93
1:C:37:ASN:CB	1:C:39:PHE:CZ	2.50	0.93
1:A:31:LEU:O	1:A:39:PHE:HZ	1.51	0.92
1:A:31:LEU:O	1:A:39:PHE:CZ	2.21	0.92
1:B:157:LYS:NZ	1:B:166:ASN:N	2.17	0.92
1:D:31:LEU:O	1:D:39:PHE:HZ	1.51	0.92
1:C:31:LEU:O	1:C:39:PHE:CZ	2.21	0.92
1:C:157:LYS:NZ	1:C:166:ASN:N	2.17	0.91
1:D:157:LYS:NZ	1:D:166:ASN:N	2.17	0.91
1:A:157:LYS:NZ	1:A:166:ASN:N	2.17	0.91
1:D:265:LEU:CG	1:D:269:GLU:CB	2.30	0.90
1:A:31:LEU:C	1:A:39:PHE:CZ	2.50	0.90
1:C:31:LEU:C	1:C:39:PHE:CZ	2.50	0.90
1:A:32:ALA:HA	1:A:39:PHE:HE2	1.04	0.90
1:B:157:LYS:HZ2	1:B:166:ASN:H	1.16	0.90
1:D:31:LEU:C	1:D:39:PHE:CZ	2.50	0.89
1:B:265:LEU:CD2	1:B:269:GLU:CB	2.50	0.89
1:B:37:ASN:CB	1:B:39:PHE:CZ	2.50	0.89
1:C:265:LEU:CD2	1:C:269:GLU:HB2	2.03	0.89
1:B:31:LEU:C	1:B:39:PHE:CZ	2.50	0.89
1:B:265:LEU:CD2	1:B:269:GLU:HB2	2.03	0.89
1:D:37:ASN:HB2	1:D:39:PHE:HZ	1.37	0.88
1:D:265:LEU:CD2	1:D:269:GLU:CB	2.51	0.88
1:A:265:LEU:CD2	1:A:269:GLU:CB	2.51	0.88
1:D:265:LEU:CD2	1:D:269:GLU:HB2	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:LEU:CD2	1:C:269:GLU:CB	2.51	0.88
1:A:265:LEU:CD2	1:A:269:GLU:HB2	2.03	0.88
1:C:157:LYS:HZ3	1:C:167:SER:H	1.23	0.87
1:B:157:LYS:HZ3	1:B:167:SER:H	1.19	0.87
1:C:157:LYS:HZ2	1:C:166:ASN:H	1.21	0.86
1:D:32:ALA:HA	1:D:39:PHE:HE2	1.04	0.85
1:A:61:LEU:HD21	1:A:104:ILE:CG2	2.07	0.84
1:C:61:LEU:HD21	1:C:104:ILE:CG2	2.07	0.84
1:D:61:LEU:HD21	1:D:104:ILE:CG2	2.07	0.84
1:C:37:ASN:HB2	1:C:39:PHE:HZ	1.37	0.84
1:C:61:LEU:HD21	1:C:104:ILE:HG21	1.60	0.84
1:B:265:LEU:CD1	1:B:269:GLU:HB3	1.82	0.83
1:B:61:LEU:HD21	1:B:104:ILE:HG21	1.60	0.83
1:B:61:LEU:HD21	1:B:104:ILE:CG2	2.07	0.83
1:D:157:LYS:HZ2	1:D:166:ASN:H	1.23	0.83
1:D:157:LYS:HZ3	1:D:167:SER:H	1.24	0.83
1:D:61:LEU:HD21	1:D:104:ILE:HG21	1.60	0.83
1:C:265:LEU:HG	1:C:266:SER:N	1.94	0.82
1:A:61:LEU:HD21	1:A:104:ILE:HG21	1.60	0.82
1:C:32:ALA:HA	1:C:39:PHE:HE2	1.04	0.81
1:B:265:LEU:HG	1:B:266:SER:N	1.94	0.81
1:B:265:LEU:CD2	1:B:270:LEU:N	2.44	0.81
1:C:265:LEU:CD2	1:C:270:LEU:N	2.44	0.81
1:D:265:LEU:CD2	1:D:270:LEU:N	2.44	0.80
1:A:265:LEU:CD2	1:A:270:LEU:N	2.44	0.80
1:B:37:ASN:HB2	1:B:39:PHE:HZ	1.38	0.79
1:D:265:LEU:HG	1:D:266:SER:N	1.94	0.79
1:B:265:LEU:HD11	1:B:269:GLU:CD	2.08	0.79
1:A:37:ASN:HB2	1:A:39:PHE:HZ	1.37	0.79
1:C:265:LEU:CD1	1:C:269:GLU:HB3	1.82	0.79
1:D:265:LEU:HD11	1:D:269:GLU:CD	2.08	0.79
1:A:265:LEU:HD11	1:A:269:GLU:CD	2.08	0.78
1:B:265:LEU:CD1	1:B:269:GLU:CG	2.45	0.77
1:C:265:LEU:HD11	1:C:269:GLU:CD	2.08	0.77
1:B:61:LEU:HD22	1:B:108:LEU:HD11	1.68	0.76
1:C:61:LEU:HD22	1:C:108:LEU:HD11	1.68	0.76
1:C:265:LEU:CD1	1:C:269:GLU:CG	2.45	0.75
1:A:265:LEU:CD1	1:A:269:GLU:CG	2.45	0.75
1:A:265:LEU:HG	1:A:266:SER:N	1.94	0.75
1:A:265:LEU:HD23	1:A:270:LEU:N	2.02	0.75
1:A:61:LEU:HD22	1:A:108:LEU:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:HD22	1:D:108:LEU:HD11	1.68	0.74
1:D:265:LEU:HD23	1:D:270:LEU:N	2.02	0.74
1:A:262:GLU:CD	1:A:360:GLN:NE2	2.45	0.74
1:C:262:GLU:CD	1:C:360:GLN:NE2	2.45	0.74
1:C:157:LYS:NZ	1:C:165:ASP:OD1	2.19	0.74
1:D:265:LEU:CD1	1:D:269:GLU:CG	2.45	0.73
1:B:262:GLU:CD	1:B:360:GLN:NE2	2.45	0.73
1:D:265:LEU:CD1	1:D:269:GLU:HB3	1.82	0.73
1:D:262:GLU:CD	1:D:360:GLN:NE2	2.45	0.73
1:C:265:LEU:HD23	1:C:270:LEU:N	2.02	0.73
1:B:265:LEU:HD23	1:B:270:LEU:N	2.02	0.72
1:A:157:LYS:NZ	1:A:165:ASP:OD1	2.19	0.72
1:C:262:GLU:CD	1:C:360:GLN:HE22	1.97	0.72
1:B:157:LYS:NZ	1:B:165:ASP:OD1	2.19	0.72
1:D:157:LYS:NZ	1:D:165:ASP:OD1	2.19	0.72
1:D:265:LEU:HD21	1:D:269:GLU:O	1.90	0.71
1:A:265:LEU:CD1	1:A:269:GLU:HB3	1.82	0.71
1:C:265:LEU:HD21	1:C:269:GLU:O	1.90	0.71
1:B:376:VAL:HG12	1:B:392:VAL:HG21	1.73	0.70
1:C:376:VAL:HG12	1:C:392:VAL:HG21	1.73	0.70
1:D:376:VAL:HG12	1:D:392:VAL:HG21	1.73	0.70
1:B:265:LEU:HD21	1:B:269:GLU:O	1.90	0.70
1:A:157:LYS:HZ3	1:A:167:SER:N	1.89	0.69
1:B:262:GLU:CD	1:B:360:GLN:HE22	1.97	0.69
1:A:37:ASN:HB2	1:A:39:PHE:CE2	2.23	0.69
1:A:262:GLU:CD	1:A:360:GLN:HE22	1.97	0.69
1:A:376:VAL:HG12	1:A:392:VAL:HG21	1.73	0.69
1:C:265:LEU:CG	1:C:266:SER:H	2.00	0.68
1:B:121:TRP:HB2	1:B:125:ILE:HD13	1.75	0.68
1:A:246:LEU:HD13	1:A:285:ILE:HD11	1.76	0.68
1:A:121:TRP:HB2	1:A:125:ILE:HD13	1.75	0.68
1:B:37:ASN:HB2	1:B:39:PHE:CE2	2.23	0.68
1:B:246:LEU:HD13	1:B:285:ILE:HD11	1.76	0.68
1:D:262:GLU:CD	1:D:360:GLN:HE22	1.97	0.68
1:C:37:ASN:HB2	1:C:39:PHE:CE2	2.23	0.68
1:C:121:TRP:HB2	1:C:125:ILE:HD13	1.75	0.68
1:D:265:LEU:CD1	1:D:269:GLU:CD	2.67	0.68
1:A:265:LEU:CD1	1:A:269:GLU:CD	2.67	0.67
1:D:37:ASN:HB2	1:D:39:PHE:CE2	2.23	0.67
1:D:157:LYS:HD2	1:D:166:ASN:HB3	1.77	0.67
1:D:246:LEU:HD13	1:D:285:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD21	1:A:269:GLU:O	1.90	0.67
1:A:157:LYS:HD2	1:A:166:ASN:HB3	1.77	0.67
1:C:157:LYS:HD2	1:C:166:ASN:HB3	1.76	0.67
1:C:265:LEU:CD1	1:C:269:GLU:CD	2.67	0.67
1:D:121:TRP:HB2	1:D:125:ILE:HD13	1.75	0.67
1:C:246:LEU:HD13	1:C:285:ILE:HD11	1.76	0.67
1:B:157:LYS:HD2	1:B:166:ASN:HB3	1.76	0.65
1:C:157:LYS:NZ	1:C:166:ASN:H	1.87	0.65
1:B:265:LEU:CD1	1:B:269:GLU:CD	2.67	0.65
1:B:157:LYS:HZ3	1:B:167:SER:N	1.92	0.65
1:A:160:PHE:CE1	1:A:207:LYS:HD2	2.33	0.64
1:B:160:PHE:CE1	1:B:207:LYS:HD2	2.33	0.64
1:D:160:PHE:CE1	1:D:207:LYS:HD2	2.33	0.64
1:C:157:LYS:HZ3	1:C:167:SER:N	1.94	0.63
1:C:160:PHE:CE1	1:C:207:LYS:HD2	2.33	0.63
1:D:157:LYS:HZ3	1:D:167:SER:N	1.95	0.63
1:D:307:VAL:HG12	1:D:307:VAL:O	1.99	0.63
1:A:307:VAL:HG12	1:A:307:VAL:O	1.99	0.63
1:B:307:VAL:HG12	1:B:307:VAL:O	1.99	0.62
1:C:307:VAL:HG12	1:C:307:VAL:O	1.99	0.62
1:C:61:LEU:HD21	1:C:104:ILE:HG23	1.81	0.62
1:A:265:LEU:CG	1:A:266:SER:H	2.00	0.61
1:D:61:LEU:HD21	1:D:104:ILE:HG23	1.81	0.61
1:C:249:ARG:HH21	1:C:310:ARG:HB3	1.66	0.61
1:A:61:LEU:HD21	1:A:104:ILE:HG23	1.81	0.61
1:B:249:ARG:HH21	1:B:310:ARG:HB3	1.66	0.61
1:D:249:ARG:HH21	1:D:310:ARG:HB3	1.66	0.60
1:D:157:LYS:NZ	1:D:167:SER:H	1.98	0.60
1:B:249:ARG:NH2	1:B:310:ARG:HB3	2.17	0.60
1:B:363:ASN:O	1:B:366:LEU:HB3	2.02	0.60
1:D:363:ASN:O	1:D:366:LEU:HB3	2.02	0.60
1:A:363:ASN:O	1:A:366:LEU:HB3	2.02	0.59
1:D:157:LYS:NZ	1:D:166:ASN:H	1.87	0.59
1:A:249:ARG:HH21	1:A:310:ARG:HB3	1.66	0.59
1:A:182:LEU:O	1:A:186:ILE:HD12	2.03	0.59
1:A:249:ARG:NH2	1:A:310:ARG:HB3	2.17	0.59
1:D:182:LEU:O	1:D:186:ILE:HD12	2.03	0.59
1:D:249:ARG:NH2	1:D:310:ARG:HB3	2.17	0.59
1:C:249:ARG:NH2	1:C:310:ARG:HB3	2.17	0.58
1:C:363:ASN:O	1:C:366:LEU:HB3	2.02	0.58
1:B:182:LEU:O	1:B:186:ILE:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:LYS:HZ3	1:D:166:ASN:N	2.00	0.58
1:C:182:LEU:O	1:C:186:ILE:HD12	2.03	0.58
1:B:61:LEU:HD21	1:B:104:ILE:HG23	1.82	0.57
1:B:157:LYS:NZ	1:B:167:SER:H	1.98	0.57
1:A:157:LYS:NZ	1:A:166:ASN:H	1.87	0.57
1:C:61:LEU:HD22	1:C:108:LEU:CD1	2.35	0.56
1:C:157:LYS:NZ	1:C:167:SER:H	1.98	0.56
1:C:166:ASN:O	1:C:167:SER:C	2.48	0.56
1:D:166:ASN:O	1:D:167:SER:C	2.48	0.56
1:C:157:LYS:HZ3	1:C:166:ASN:N	2.03	0.56
1:B:157:LYS:NZ	1:B:166:ASN:H	1.87	0.56
1:D:157:LYS:HZ2	1:D:165:ASP:C	2.14	0.56
1:D:61:LEU:HD22	1:D:108:LEU:CD1	2.35	0.56
1:B:333:VAL:HA	1:B:352:ILE:HB	1.88	0.55
1:C:333:VAL:HA	1:C:352:ILE:HB	1.88	0.55
1:B:61:LEU:HD22	1:B:108:LEU:CD1	2.35	0.55
1:A:333:VAL:HA	1:A:352:ILE:HB	1.88	0.55
1:B:166:ASN:O	1:B:167:SER:C	2.48	0.55
1:A:166:ASN:O	1:A:167:SER:C	2.48	0.55
1:D:333:VAL:HA	1:D:352:ILE:HB	1.88	0.55
1:B:32:ALA:HB2	1:B:39:PHE:CD2	2.42	0.54
1:B:353:ALA:HB3	1:B:375:GLU:HA	1.90	0.54
1:A:32:ALA:HB2	1:A:39:PHE:CD2	2.42	0.54
1:D:353:ALA:HB3	1:D:375:GLU:HA	1.90	0.54
1:D:32:ALA:HB2	1:D:39:PHE:CD2	2.42	0.54
1:A:353:ALA:HB3	1:A:375:GLU:HA	1.90	0.53
1:C:32:ALA:HB2	1:C:39:PHE:CD2	2.42	0.53
1:C:353:ALA:HB3	1:C:375:GLU:HA	1.90	0.53
1:B:246:LEU:HD13	1:B:285:ILE:CD1	2.39	0.53
1:C:157:LYS:HZ2	1:C:165:ASP:C	2.14	0.53
1:A:157:LYS:HZ2	1:A:165:ASP:C	2.15	0.53
1:A:63:GLU:HG2	1:A:65:HIS:CE1	2.43	0.53
1:C:246:LEU:HD13	1:C:285:ILE:CD1	2.39	0.53
1:B:101:PHE:CD2	1:B:121:TRP:HZ3	2.27	0.53
1:B:157:LYS:HZ2	1:B:165:ASP:C	2.14	0.53
1:A:61:LEU:HD22	1:A:108:LEU:CD1	2.35	0.52
1:A:365:LYS:O	1:A:369:GLU:N	2.43	0.52
1:A:101:PHE:CD2	1:A:121:TRP:HZ3	2.27	0.52
1:D:101:PHE:CD2	1:D:121:TRP:HZ3	2.27	0.52
1:D:246:LEU:HD13	1:D:285:ILE:CD1	2.39	0.52
1:C:119:PRO:O	1:C:121:TRP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HD23	1:C:221:VAL:HB	1.92	0.52
1:B:197:LEU:HD23	1:B:221:VAL:HB	1.92	0.52
1:B:365:LYS:O	1:B:369:GLU:N	2.43	0.52
1:C:101:PHE:CD2	1:C:121:TRP:HZ3	2.27	0.52
1:A:197:LEU:HD23	1:A:221:VAL:HB	1.92	0.51
1:D:197:LEU:HD23	1:D:221:VAL:HB	1.92	0.51
1:D:119:PRO:O	1:D:121:TRP:N	2.43	0.51
1:A:246:LEU:HD13	1:A:285:ILE:CD1	2.39	0.51
1:B:265:LEU:HD23	1:B:270:LEU:CA	2.41	0.51
1:A:53:LYS:HG3	1:A:54:ASP:H	1.76	0.51
1:B:53:LYS:HG3	1:B:54:ASP:H	1.76	0.51
1:A:119:PRO:O	1:A:121:TRP:N	2.43	0.50
1:C:265:LEU:HD23	1:C:270:LEU:CA	2.41	0.50
1:D:122:ALA:N	1:D:123:PRO:HD2	2.27	0.50
1:D:157:LYS:HZ2	1:D:165:ASP:HA	1.77	0.50
1:B:122:ALA:N	1:B:123:PRO:HD2	2.27	0.50
1:C:122:ALA:N	1:C:123:PRO:HD2	2.27	0.50
1:D:53:LYS:HG3	1:D:54:ASP:H	1.76	0.50
1:A:122:ALA:N	1:A:123:PRO:HD2	2.27	0.50
1:C:365:LYS:O	1:C:369:GLU:N	2.43	0.50
1:A:265:LEU:HD23	1:A:270:LEU:CA	2.41	0.50
1:A:426:ARG:HA	1:A:429:GLU:HG2	1.93	0.50
1:C:31:LEU:HB2	1:C:39:PHE:CE1	2.47	0.50
1:B:31:LEU:HB2	1:B:39:PHE:CE1	2.46	0.50
1:D:426:ARG:HA	1:D:429:GLU:HG2	1.93	0.50
1:D:31:LEU:HB2	1:D:39:PHE:CE1	2.47	0.50
1:B:426:ARG:HA	1:B:429:GLU:HG2	1.93	0.49
1:D:365:LYS:O	1:D:369:GLU:N	2.43	0.49
1:C:53:LYS:HG3	1:C:54:ASP:H	1.76	0.49
1:D:265:LEU:HD23	1:D:270:LEU:CA	2.41	0.49
1:A:31:LEU:HB2	1:A:39:PHE:CE1	2.47	0.49
1:B:414:GLU:O	1:B:418:GLU:N	2.46	0.49
1:C:414:GLU:O	1:C:418:GLU:N	2.46	0.49
1:C:426:ARG:HA	1:C:429:GLU:HG2	1.93	0.49
1:B:157:LYS:NZ	1:B:165:ASP:C	2.71	0.48
1:C:157:LYS:HZ2	1:C:165:ASP:HA	1.78	0.48
1:C:157:LYS:NZ	1:C:165:ASP:C	2.71	0.48
1:A:414:GLU:O	1:A:418:GLU:N	2.46	0.48
1:B:32:ALA:N	1:B:39:PHE:CE2	2.82	0.48
1:C:12:LEU:HD11	1:C:114:ILE:HD12	1.96	0.48
1:A:125:ILE:O	1:A:129:HIS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:NZ	1:A:165:ASP:C	2.71	0.47
1:D:12:LEU:HD11	1:D:114:ILE:HD12	1.96	0.47
1:D:414:GLU:O	1:D:418:GLU:N	2.46	0.47
1:B:119:PRO:O	1:B:121:TRP:N	2.43	0.47
1:A:12:LEU:HD11	1:A:114:ILE:HD12	1.96	0.47
1:B:157:LYS:HZ3	1:B:166:ASN:N	2.07	0.47
1:D:125:ILE:O	1:D:129:HIS:HD2	1.97	0.47
1:D:157:LYS:NZ	1:D:165:ASP:C	2.71	0.47
1:A:93:ALA:O	1:A:96:THR:N	2.43	0.47
1:B:12:LEU:HD11	1:B:114:ILE:HD12	1.96	0.47
1:B:125:ILE:O	1:B:129:HIS:HD2	1.97	0.47
1:D:265:LEU:CG	1:D:266:SER:H	2.00	0.47
1:C:32:ALA:N	1:C:39:PHE:CE2	2.83	0.47
1:B:93:ALA:O	1:B:96:THR:N	2.43	0.47
1:C:125:ILE:O	1:C:129:HIS:HD2	1.97	0.47
1:D:32:ALA:N	1:D:39:PHE:CE2	2.82	0.47
1:A:32:ALA:N	1:A:39:PHE:CE2	2.82	0.46
1:B:433:GLN:HA	1:B:436:LYS:HG2	1.98	0.46
1:C:433:GLN:HA	1:C:436:LYS:HG2	1.98	0.46
1:C:14:PRO:HB3	1:C:24:PHE:CG	2.51	0.46
1:A:14:PRO:HB3	1:A:24:PHE:CG	2.51	0.46
1:A:265:LEU:CG	1:A:266:SER:N	2.68	0.46
1:C:93:ALA:O	1:C:96:THR:N	2.43	0.46
1:C:157:LYS:CD	1:C:166:ASN:HB3	2.46	0.45
1:D:157:LYS:CD	1:D:166:ASN:HB3	2.46	0.45
1:B:14:PRO:HB3	1:B:24:PHE:CG	2.51	0.45
1:B:61:LEU:HD21	1:B:104:ILE:HD13	1.98	0.45
1:C:61:LEU:HD21	1:C:104:ILE:HD13	1.98	0.45
1:D:14:PRO:HB3	1:D:24:PHE:CG	2.51	0.45
1:D:47:LEU:O	1:D:50:ILE:HG22	2.17	0.45
1:A:30:GLN:O	1:A:34:ARG:HG2	2.17	0.45
1:A:433:GLN:HA	1:A:436:LYS:HG2	1.98	0.45
1:C:263:TYR:C	1:C:265:LEU:H	2.25	0.45
1:A:47:LEU:O	1:A:50:ILE:HG22	2.17	0.45
1:D:61:LEU:HD21	1:D:104:ILE:HD13	1.98	0.45
1:D:213:SER:HA	1:D:220:LEU:HD23	1.99	0.45
1:D:307:VAL:O	1:D:307:VAL:CG1	2.65	0.45
1:A:213:SER:HA	1:A:220:LEU:HD23	1.99	0.45
1:D:263:TYR:C	1:D:265:LEU:H	2.25	0.45
1:B:47:LEU:O	1:B:50:ILE:HG22	2.17	0.45
1:B:263:TYR:C	1:B:265:LEU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:GLN:O	1:D:34:ARG:HG2	2.17	0.45
1:D:31:LEU:C	1:D:39:PHE:CE2	2.95	0.45
1:D:265:LEU:CG	1:D:266:SER:N	2.68	0.45
1:D:433:GLN:HA	1:D:436:LYS:HG2	1.98	0.44
1:B:30:GLN:O	1:B:34:ARG:HG2	2.17	0.44
1:B:213:SER:HA	1:B:220:LEU:HD23	1.99	0.44
1:C:47:LEU:O	1:C:50:ILE:HG22	2.17	0.44
1:A:263:TYR:C	1:A:265:LEU:H	2.25	0.44
1:C:265:LEU:CD2	1:C:269:GLU:HB3	2.44	0.44
1:A:332:PHE:HD2	1:A:344:SER:HB2	1.83	0.44
1:B:32:ALA:CB	1:B:39:PHE:CD2	3.01	0.44
1:C:236:ASP:O	1:C:239:THR:HG22	2.18	0.44
1:C:307:VAL:O	1:C:307:VAL:CG1	2.65	0.44
1:D:32:ALA:CB	1:D:39:PHE:CD2	3.01	0.44
1:A:61:LEU:HD21	1:A:104:ILE:HD13	1.98	0.44
1:B:157:LYS:HZ2	1:B:165:ASP:HA	1.83	0.44
1:C:30:GLN:O	1:C:34:ARG:HG2	2.17	0.44
1:C:213:SER:HA	1:C:220:LEU:HD23	1.99	0.44
1:A:265:LEU:CD2	1:A:269:GLU:HB3	2.44	0.44
1:C:31:LEU:C	1:C:39:PHE:CE2	2.95	0.44
1:D:236:ASP:O	1:D:239:THR:HG22	2.18	0.44
1:D:332:PHE:HD2	1:D:344:SER:HB2	1.83	0.44
1:A:157:LYS:CD	1:A:166:ASN:HB3	2.46	0.44
1:A:236:ASP:O	1:A:239:THR:HG22	2.18	0.43
1:C:32:ALA:CB	1:C:39:PHE:CD2	3.01	0.43
1:B:51:LYS:HD3	1:B:51:LYS:HA	1.78	0.43
1:B:157:LYS:CD	1:B:166:ASN:HB3	2.46	0.43
1:A:263:TYR:O	1:A:263:TYR:CD1	2.72	0.43
1:B:236:ASP:O	1:B:239:THR:HG22	2.18	0.43
1:D:263:TYR:O	1:D:263:TYR:CD1	2.72	0.43
1:A:32:ALA:CB	1:A:39:PHE:CD2	3.01	0.43
1:A:25:PHE:CE2	1:A:29:LYS:HD2	2.53	0.43
1:D:25:PHE:CE2	1:D:29:LYS:HD2	2.53	0.43
1:D:157:LYS:HZ2	1:D:165:ASP:CA	2.30	0.43
1:A:262:GLU:OE2	1:A:360:GLN:NE2	2.52	0.43
1:C:332:PHE:HD2	1:C:344:SER:HB2	1.83	0.43
1:A:306:ARG:HD2	1:A:306:ARG:HA	1.81	0.43
1:B:31:LEU:C	1:B:39:PHE:CE2	2.95	0.43
1:B:263:TYR:CD1	1:B:263:TYR:O	2.72	0.43
1:B:332:PHE:HD2	1:B:344:SER:HB2	1.83	0.43
1:B:262:GLU:OE2	1:B:360:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:PHE:CE2	1:C:29:LYS:HD2	2.53	0.43
1:D:262:GLU:OE2	1:D:360:GLN:NE2	2.52	0.43
1:B:307:VAL:O	1:B:307:VAL:CG1	2.65	0.42
1:C:157:LYS:HZ2	1:C:165:ASP:CA	2.32	0.42
1:C:263:TYR:O	1:C:263:TYR:CD1	2.72	0.42
1:D:265:LEU:HD21	1:D:269:GLU:HB3	1.94	0.42
1:B:25:PHE:CE2	1:B:29:LYS:HD2	2.53	0.42
1:C:262:GLU:OE2	1:C:360:GLN:NE2	2.52	0.42
1:D:122:ALA:HB3	1:D:123:PRO:HD3	2.02	0.42
1:A:50:ILE:HD12	1:A:50:ILE:HA	1.87	0.42
1:A:122:ALA:HB3	1:A:123:PRO:HD3	2.02	0.42
1:A:394:ARG:O	1:A:399:GLU:HB2	2.20	0.42
1:A:31:LEU:O	1:A:39:PHE:CE2	2.71	0.42
1:B:122:ALA:HB3	1:B:123:PRO:HD3	2.02	0.41
1:D:394:ARG:O	1:D:399:GLU:HB2	2.20	0.41
1:B:394:ARG:O	1:B:399:GLU:HB2	2.20	0.41
1:B:365:LYS:HA	1:B:368:ALA:HB3	2.02	0.41
1:B:403:GLU:O	1:B:404:VAL:C	2.64	0.41
1:C:31:LEU:O	1:C:39:PHE:CE2	2.71	0.41
1:C:265:LEU:HD23	1:C:270:LEU:HA	2.03	0.41
1:C:394:ARG:O	1:C:399:GLU:HB2	2.20	0.41
1:D:93:ALA:O	1:D:96:THR:N	2.43	0.41
1:A:304:VAL:C	1:A:306:ARG:H	2.29	0.41
1:A:307:VAL:O	1:A:307:VAL:CG1	2.65	0.41
1:A:365:LYS:HA	1:A:368:ALA:HB3	2.02	0.41
1:C:362:LEU:HD22	1:C:362:LEU:H	1.86	0.41
1:D:32:ALA:CB	1:D:39:PHE:CE2	3.04	0.41
1:A:31:LEU:C	1:A:39:PHE:CE2	2.95	0.41
1:C:122:ALA:HB3	1:C:123:PRO:HD3	2.02	0.41
1:D:265:LEU:HD23	1:D:270:LEU:HA	2.03	0.41
1:D:365:LYS:HA	1:D:368:ALA:HB3	2.02	0.41
1:B:265:LEU:HD23	1:B:270:LEU:HA	2.03	0.41
1:B:362:LEU:H	1:B:362:LEU:HD22	1.86	0.41
1:C:51:LYS:HA	1:C:51:LYS:HD3	1.78	0.41
1:A:32:ALA:CB	1:A:39:PHE:CE2	3.04	0.40
1:B:31:LEU:O	1:B:39:PHE:CE2	2.71	0.40
1:B:21:ILE:HD11	1:B:47:LEU:HD23	2.03	0.40
1:B:124:GLU:H	1:B:124:GLU:HG3	1.71	0.40
1:C:105:LEU:O	1:C:109:ASN:N	2.51	0.40
1:C:365:LYS:HA	1:C:368:ALA:HB3	2.02	0.40
1:D:246:LEU:HD12	1:D:254:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:LEU:HD22	1:D:362:LEU:H	1.86	0.40
1:D:403:GLU:O	1:D:404:VAL:C	2.64	0.40
1:A:21:ILE:HD11	1:A:47:LEU:HD23	2.03	0.40
1:A:246:LEU:HD12	1:A:254:VAL:HG21	2.02	0.40
1:C:122:ALA:HB3	1:C:123:PRO:CD	2.52	0.40
1:C:251:GLU:HA	1:C:328:SER:HA	2.03	0.40
1:A:122:ALA:HB3	1:A:123:PRO:CD	2.52	0.40
1:A:265:LEU:HD21	1:A:269:GLU:HB3	1.94	0.40
1:B:158:TYR:HA	1:B:159:PRO:HD3	1.92	0.40
1:C:27:LEU:O	1:C:31:LEU:HG	2.22	0.40
1:C:246:LEU:HD12	1:C:254:VAL:HG21	2.02	0.40
1:D:122:ALA:HB3	1:D:123:PRO:CD	2.52	0.40
1:A:265:LEU:HD23	1:A:270:LEU:HA	2.03	0.40
1:A:362:LEU:HD22	1:A:362:LEU:H	1.86	0.40
1:D:21:ILE:HD11	1:D:47:LEU:HD23	2.03	0.40
1:D:105:LEU:O	1:D:109:ASN:N	2.51	0.40

All (27) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:CD1	1:D:156:GLU:OE1[1_455]	1.09	1.11
1:B:64:LEU:CD1	1:B:156:GLU:OE1[1_455]	1.10	1.10
1:A:64:LEU:CD2	1:A:156:GLU:OE1[1_655]	1.17	1.03
1:A:64:LEU:CB	1:A:156:GLU:OE2[1_655]	1.36	0.84
1:B:414:GLU:OE2	1:D:33:LYS:NZ[1_565]	1.39	0.81
1:C:64:LEU:CD1	1:C:156:GLU:OE1[1_655]	1.39	0.81
1:B:64:LEU:CA	1:B:156:GLU:OE2[1_455]	1.46	0.74
1:D:64:LEU:CA	1:D:156:GLU:OE2[1_455]	1.47	0.73
1:A:64:LEU:CA	1:A:156:GLU:OE2[1_655]	1.57	0.63
1:A:306:ARG:NH2	1:B:305:GLN:CB[1_654]	1.69	0.51
1:C:64:LEU:CA	1:C:156:GLU:OE2[1_655]	1.69	0.51
1:B:414:GLU:OE2	1:D:33:LYS:CE[1_565]	1.70	0.50
1:C:64:LEU:C	1:C:156:GLU:OE2[1_655]	1.72	0.48
1:B:64:LEU:CB	1:B:156:GLU:OE2[1_455]	1.75	0.45
1:D:64:LEU:CB	1:D:156:GLU:OE2[1_455]	1.77	0.43
1:C:65:HIS:N	1:C:156:GLU:OE2[1_655]	1.78	0.42
1:B:64:LEU:C	1:B:156:GLU:OE2[1_455]	1.85	0.35
1:C:64:LEU:CB	1:C:156:GLU:OE2[1_655]	1.86	0.34
1:D:64:LEU:C	1:D:156:GLU:OE2[1_455]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:N	1:B:156:GLU:OE2[1_455]	1.97	0.23
1:D:65:HIS:N	1:D:156:GLU:OE2[1_455]	1.99	0.21
1:A:64:LEU:CG	1:A:156:GLU:OE1[1_655]	2.02	0.18
1:A:64:LEU:CB	1:A:156:GLU:CD[1_655]	2.03	0.17
1:A:64:LEU:C	1:A:156:GLU:OE2[1_655]	2.08	0.12
1:C:64:LEU:CG	1:C:156:GLU:OE1[1_655]	2.13	0.07
1:B:64:LEU:CG	1:B:156:GLU:OE1[1_455]	2.17	0.03
1:B:414:GLU:CD	1:D:33:LYS:NZ[1_565]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/455 (81%)	339 (92%)	29 (8%)	0	100	100
1	B	368/455 (81%)	337 (92%)	31 (8%)	0	100	100
1	C	368/455 (81%)	337 (92%)	31 (8%)	0	100	100
1	D	368/455 (81%)	337 (92%)	31 (8%)	0	100	100
All	All	1472/1820 (81%)	1350 (92%)	122 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/396 (83%)	325 (99%)	2 (1%)	78	93
1	B	327/396 (83%)	327 (100%)	0	100	100
1	C	327/396 (83%)	327 (100%)	0	100	100
1	D	327/396 (83%)	327 (100%)	0	100	100
All	All	1308/1584 (83%)	1306 (100%)	2 (0%)	87	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	381	ASN
1	B	381	ASN
1	C	130	ASN
1	C	381	ASN
1	D	381	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/455 (83%)	1.24	78 (20%) 2 2	30, 57, 104, 143	0
1	B	378/455 (83%)	1.69	128 (33%) 1 1	33, 63, 116, 156	0
1	C	378/455 (83%)	1.77	138 (36%) 1 0	30, 65, 112, 169	0
1	D	378/455 (83%)	1.93	149 (39%) 1 0	37, 73, 129, 157	0
All	All	1512/1820 (83%)	1.66	493 (32%) 1 1	30, 64, 118, 169	0

All (493) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	313	VAL	7.3
1	C	237	PRO	7.3
1	C	251	GLU	7.2
1	D	45	ILE	7.0
1	C	263	TYR	6.6
1	D	39	PHE	6.4
1	B	442	GLN	6.4
1	B	43	THR	6.2
1	C	43	THR	6.1
1	C	63	GLU	6.0
1	D	384	TYR	5.9
1	B	368	ALA	5.9
1	D	318	ALA	5.7
1	B	45	ILE	5.6
1	A	442	GLN	5.5
1	C	422	GLN	5.2
1	C	382	GLY	5.1
1	D	43	THR	5.1
1	C	35	ASN	5.1
1	D	63	GLU	5.1
1	A	43	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	45	ILE	5.0
1	A	45	ILE	5.0
1	B	263	TYR	5.0
1	B	54	ASP	5.0
1	D	288	VAL	4.9
1	D	147	GLY	4.8
1	D	240	GLU	4.8
1	C	381	ASN	4.8
1	A	161	PRO	4.7
1	D	194	ASP	4.7
1	D	227	VAL	4.7
1	A	288	VAL	4.6
1	C	442	GLN	4.6
1	D	18	HIS	4.6
1	C	309	ASP	4.5
1	D	376	VAL	4.5
1	A	264	PHE	4.5
1	D	309	ASP	4.5
1	D	304	VAL	4.4
1	B	39	PHE	4.4
1	B	403	GLU	4.4
1	B	19	GLY	4.4
1	D	312	LEU	4.3
1	D	442	GLN	4.3
1	C	236	ASP	4.3
1	C	440	ASP	4.3
1	D	303	PHE	4.2
1	C	356	ARG	4.1
1	C	179	MET	4.1
1	C	127	SER	4.1
1	B	413	SER	4.1
1	B	18	HIS	4.0
1	B	313	VAL	4.0
1	C	46	ASN	4.0
1	C	331	GLY	4.0
1	A	273	VAL	4.0
1	C	392	VAL	4.0
1	B	440	ASP	3.9
1	C	379	ASP	3.9
1	A	381	ASN	3.9
1	D	54	ASP	3.9
1	D	236	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	281	THR	3.9
1	C	50	ILE	3.9
1	D	286	TRP	3.9
1	B	273	VAL	3.9
1	C	182	LEU	3.8
1	C	312	LEU	3.8
1	A	39	PHE	3.8
1	B	256	PHE	3.8
1	B	217	ASP	3.8
1	D	316	GLY	3.8
1	C	156	GLU	3.8
1	A	262	GLU	3.7
1	D	264	PHE	3.7
1	D	242	ILE	3.7
1	B	61	LEU	3.7
1	B	64	LEU	3.7
1	B	308	GLY	3.7
1	C	48	SER	3.7
1	D	317	TRP	3.7
1	B	371	GLY	3.7
1	C	238	LYS	3.7
1	B	91	ARG	3.6
1	B	303	PHE	3.6
1	B	317	TRP	3.6
1	D	441	GLU	3.6
1	A	181	LEU	3.6
1	D	44	PRO	3.6
1	D	277	LEU	3.6
1	B	94	PHE	3.6
1	D	308	GLY	3.6
1	B	384	TYR	3.6
1	B	237	PRO	3.6
1	C	264	PHE	3.6
1	D	263	TYR	3.6
1	D	412	LEU	3.5
1	D	239	THR	3.5
1	B	284	PHE	3.5
1	D	388	GLY	3.5
1	B	312	LEU	3.5
1	B	238	LYS	3.5
1	B	309	ASP	3.5
1	B	243	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	382	GLY	3.5
1	C	377	VAL	3.5
1	A	63	GLU	3.5
1	C	380	GLU	3.5
1	D	324	LEU	3.5
1	C	210	ASP	3.5
1	C	317	TRP	3.5
1	D	371	GLY	3.4
1	B	239	THR	3.4
1	D	250	ALA	3.4
1	B	60	LYS	3.4
1	C	180	LYS	3.4
1	D	62	VAL	3.4
1	B	280	SER	3.4
1	D	8	ILE	3.4
1	D	155	GLY	3.4
1	C	242	ILE	3.4
1	B	265	LEU	3.3
1	D	314	VAL	3.3
1	D	397	VAL	3.3
1	C	315	GLU	3.3
1	C	143	SER	3.3
1	B	377	VAL	3.3
1	D	46	ASN	3.3
1	C	248	LYS	3.3
1	D	358	LEU	3.3
1	B	359	ASP	3.3
1	C	8	ILE	3.3
1	A	304	VAL	3.3
1	C	261	SER	3.3
1	D	237	PRO	3.3
1	B	179	MET	3.3
1	D	396	VAL	3.3
1	C	239	THR	3.3
1	D	345	MET	3.2
1	C	305	GLN	3.2
1	D	307	VAL	3.2
1	C	383	LYS	3.2
1	B	242	ILE	3.2
1	C	57	ALA	3.2
1	B	156	GLU	3.2
1	C	167	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	383	LYS	3.2
1	B	304	VAL	3.2
1	D	253	THR	3.2
1	D	271	GLU	3.2
1	A	263	TYR	3.1
1	D	332	PHE	3.1
1	C	418	GLU	3.1
1	D	156	GLU	3.1
1	A	237	PRO	3.1
1	D	417	LYS	3.1
1	A	379	ASP	3.1
1	B	35	ASN	3.1
1	C	38	VAL	3.1
1	B	8	ILE	3.1
1	D	323	ILE	3.1
1	D	319	PRO	3.1
1	B	367	ALA	3.1
1	D	321	ALA	3.0
1	C	286	TRP	3.0
1	A	165	ASP	3.0
1	D	48	SER	3.0
1	D	118	ASN	3.0
1	D	280	SER	3.0
1	D	381	ASN	3.0
1	B	373	GLY	3.0
1	B	393	ILE	3.0
1	D	251	GLU	3.0
1	D	187	ALA	3.0
1	C	62	VAL	3.0
1	C	65	HIS	3.0
1	C	55	SER	3.0
1	C	283	ASN	3.0
1	D	58	SER	3.0
1	A	36	CYS	3.0
1	D	64	LEU	3.0
1	C	160	PHE	3.0
1	B	55	SER	3.0
1	B	402	GLY	3.0
1	B	36	CYS	3.0
1	C	93	ALA	3.0
1	B	227	VAL	3.0
1	A	8	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	270	LEU	3.0
1	C	64	LEU	3.0
1	D	246	LEU	3.0
1	C	194	ASP	3.0
1	A	119	PRO	3.0
1	D	275	ILE	2.9
1	C	243	ILE	2.9
1	A	16	LEU	2.9
1	D	320	GLN	2.9
1	C	240	GLU	2.9
1	C	403	GLU	2.9
1	B	109	ASN	2.9
1	B	58	SER	2.9
1	C	327	SER	2.9
1	D	404	VAL	2.9
1	A	286	TRP	2.9
1	C	384	TYR	2.9
1	D	262	GLU	2.9
1	A	254	VAL	2.9
1	C	404	VAL	2.9
1	B	182	LEU	2.9
1	C	265	LEU	2.9
1	D	181	LEU	2.9
1	A	388	GLY	2.9
1	D	276	GLY	2.9
1	D	245	TRP	2.9
1	D	392	VAL	2.9
1	B	252	SER	2.9
1	C	303	PHE	2.9
1	C	319	PRO	2.8
1	D	305	GLN	2.8
1	B	240	GLU	2.8
1	B	251	GLU	2.8
1	B	307	VAL	2.8
1	D	273	VAL	2.8
1	C	178	ASN	2.8
1	D	270	LEU	2.8
1	C	36	CYS	2.8
1	D	382	GLY	2.8
1	D	420	GLY	2.8
1	C	97	ALA	2.8
1	D	287	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	92	ASN	2.8
1	B	381	ASN	2.8
1	D	35	ASN	2.8
1	A	182	LEU	2.8
1	A	279	ILE	2.8
1	B	389	ILE	2.8
1	C	148	LEU	2.8
1	D	383	LYS	2.8
1	C	288	VAL	2.8
1	C	376	VAL	2.8
1	D	431	LEU	2.8
1	C	398	VAL	2.8
1	D	377	VAL	2.8
1	B	277	LEU	2.8
1	B	283	ASN	2.8
1	B	379	ASP	2.8
1	B	378	ARG	2.7
1	B	441	GLU	2.7
1	D	329	THR	2.7
1	D	123	PRO	2.7
1	A	240	GLU	2.7
1	D	95	GLU	2.7
1	A	307	VAL	2.7
1	C	287	ALA	2.7
1	D	21	ILE	2.7
1	D	65	HIS	2.7
1	B	178	ASN	2.7
1	C	166	ASN	2.7
1	C	54	ASP	2.7
1	D	261	SER	2.7
1	A	305	GLN	2.7
1	A	227	VAL	2.7
1	B	351	VAL	2.7
1	A	303	PHE	2.7
1	C	141	ALA	2.7
1	C	164	TYR	2.7
1	C	110	PRO	2.7
1	D	356	ARG	2.7
1	A	380	GLU	2.7
1	D	165	ASP	2.7
1	A	377	VAL	2.7
1	B	404	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	265	LEU	2.7
1	C	393	ILE	2.6
1	D	179	MET	2.6
1	D	348	GLY	2.6
1	B	315	GLU	2.6
1	B	392	VAL	2.6
1	B	400	LYS	2.6
1	C	60	LYS	2.6
1	C	441	GLU	2.6
1	D	12	LEU	2.6
1	D	419	LYS	2.6
1	C	189	PHE	2.6
1	D	367	ALA	2.6
1	C	260	GLY	2.6
1	A	313	VAL	2.6
1	B	412	LEU	2.6
1	D	380	GLU	2.6
1	D	344	SER	2.6
1	B	65	HIS	2.6
1	D	36	CYS	2.6
1	C	151	PHE	2.6
1	A	48	SER	2.6
1	B	340	SER	2.6
1	B	253	THR	2.6
1	B	288	VAL	2.6
1	D	41	CYS	2.6
1	B	355	ALA	2.6
1	D	378	ARG	2.5
1	D	61	LEU	2.5
1	B	376	VAL	2.5
1	A	269	GLU	2.5
1	D	315	GLU	2.5
1	C	252	SER	2.5
1	B	123	PRO	2.5
1	A	384	TYR	2.5
1	C	349	VAL	2.5
1	B	390	ALA	2.5
1	D	57	ALA	2.5
1	C	249	ARG	2.5
1	C	400	LYS	2.5
1	D	162	ASP	2.5
1	B	47	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	159	PRO	2.5
1	C	277	LEU	2.5
1	C	254	VAL	2.5
1	A	441	GLU	2.5
1	A	109	ASN	2.5
1	D	37	ASN	2.5
1	A	236	ASP	2.5
1	A	108	LEU	2.5
1	B	255	VAL	2.5
1	C	411	GLU	2.5
1	B	142	ALA	2.5
1	B	287	ALA	2.5
1	C	281	THR	2.5
1	C	109	ASN	2.5
1	B	236	ASP	2.4
1	B	421	GLU	2.4
1	D	15	PHE	2.4
1	B	305	GLN	2.4
1	C	51	LYS	2.4
1	D	33	LYS	2.4
1	C	92	ASN	2.4
1	C	16	LEU	2.4
1	C	412	LEU	2.4
1	C	186	ILE	2.4
1	C	147	GLY	2.4
1	D	398	VAL	2.4
1	C	322	ARG	2.4
1	A	284	PHE	2.4
1	B	117	PHE	2.4
1	A	31	LEU	2.4
1	D	374	MET	2.4
1	A	46	ASN	2.4
1	D	119	PRO	2.4
1	D	161	PRO	2.4
1	B	397	VAL	2.4
1	C	314	VAL	2.4
1	C	316	GLY	2.4
1	D	52	ASP	2.4
1	D	284	PHE	2.4
1	D	166	ASN	2.4
1	C	304	VAL	2.4
1	C	165	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	410	ARG	2.4
1	A	317	TRP	2.4
1	B	286	TRP	2.4
1	B	115	TYR	2.4
1	B	129	HIS	2.4
1	D	16	LEU	2.4
1	B	104	ILE	2.4
1	A	44	PRO	2.4
1	A	257	VAL	2.3
1	B	314	VAL	2.3
1	B	407	ARG	2.3
1	C	378	ARG	2.3
1	D	180	LYS	2.3
1	D	385	LYS	2.3
1	C	259	PHE	2.3
1	B	380	GLU	2.3
1	C	321	ALA	2.3
1	D	22	SER	2.3
1	A	378	ARG	2.3
1	B	46	ASN	2.3
1	C	284	PHE	2.3
1	A	421	GLU	2.3
1	B	342	ALA	2.3
1	D	17	ALA	2.3
1	D	269	GLU	2.3
1	B	261	SER	2.3
1	A	281	THR	2.3
1	C	44	PRO	2.3
1	A	155	GLY	2.3
1	A	308	GLY	2.3
1	D	122	ALA	2.3
1	C	435	CYS	2.3
1	D	157	LYS	2.3
1	D	183	HIS	2.3
1	C	313	VAL	2.3
1	D	38	VAL	2.3
1	C	250	ALA	2.3
1	C	374	MET	2.3
1	C	52	ASP	2.3
1	B	245	TRP	2.3
1	A	266	SER	2.3
1	B	96	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	143	SER	2.3
1	A	287	ALA	2.2
1	A	430	GLU	2.2
1	B	181	LEU	2.2
1	B	246	LEU	2.2
1	D	346	LYS	2.2
1	D	359	ASP	2.2
1	A	50	ILE	2.2
1	C	336	CYS	2.2
1	C	96	THR	2.2
1	B	42	SER	2.2
1	B	254	VAL	2.2
1	C	119	PRO	2.2
1	C	255	VAL	2.2
1	D	143	SER	2.2
1	D	413	SER	2.2
1	B	180	LYS	2.2
1	D	226	LEU	2.2
1	A	18	HIS	2.2
1	A	356	ARG	2.2
1	B	119	PRO	2.2
1	B	159	PRO	2.2
1	A	385	LYS	2.2
1	D	178	ASN	2.2
1	A	59	ILE	2.2
1	D	322	ARG	2.2
1	C	227	VAL	2.2
1	D	372	VAL	2.2
1	C	308	GLY	2.2
1	A	277	LEU	2.2
1	C	61	LEU	2.2
1	D	205	GLU	2.2
1	A	179	MET	2.2
1	B	160	PHE	2.2
1	D	256	PHE	2.2
1	C	426	ARG	2.1
1	D	389	ILE	2.1
1	B	244	ASN	2.1
1	B	388	GLY	2.1
1	D	19	GLY	2.1
1	D	325	GLY	2.1
1	B	151	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	94	PHE	2.1
1	D	115	TYR	2.1
1	A	56	SER	2.1
1	C	58	SER	2.1
1	A	343	GLU	2.1
1	C	429	GLU	2.1
1	B	50	ILE	2.1
1	B	52	ASP	2.1
1	B	420	GLY	2.1
1	C	94	PHE	2.1
1	A	140	ALA	2.1
1	C	91	ARG	2.1
1	C	340	SER	2.1
1	B	374	MET	2.1
1	D	51	LYS	2.1
1	A	260	GLY	2.1
1	C	184	ASP	2.1
1	B	356	ARG	2.1
1	B	93	ALA	2.1
1	C	318	ALA	2.1
1	D	278	GLU	2.1
1	A	180	LYS	2.1
1	B	346	LYS	2.1
1	C	307	VAL	2.1
1	C	397	VAL	2.1
1	C	246	LEU	2.1
1	A	160	PHE	2.1
1	D	160	PHE	2.1
1	D	400	LYS	2.0
1	B	319	PRO	2.0
1	C	181	LEU	2.0
1	B	382	GLY	2.0
1	D	202	ARG	2.0
1	D	410	ARG	2.0
1	B	279	ILE	2.0
1	C	419	LYS	2.0
1	C	345	MET	2.0
1	A	62	VAL	2.0
1	A	167	SER	2.0
1	C	123	PRO	2.0
1	A	64	LEU	2.0
1	A	283	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	155	GLY	2.0
1	B	424	ILE	2.0
1	A	355	ALA	2.0
1	C	253	THR	2.0
1	D	150	ALA	2.0
1	B	63	GLU	2.0
1	D	184	ASP	2.0
1	D	440	ASP	2.0
1	A	354	MET	2.0
1	A	392	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.